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PREPARATION OF H_2O AND D_2O SLOW NEUTRON SCATTERING
KERNELS FOR ENDF USING MR TYPE MODELS

H. L. McMurry and L. J. Gannon

IDAHO NUCLEAR CORPORATION
NATIONAL REACTOR TESTING STATION
IDAHO FALLS, IDAHO

U. S. ATOMIC ENERGY COMMISSION

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IDAHO NUCLEAR CORPORATION

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ABSTRACT

This report describes the way slow neutron scattering kernels are being prepared for the Evaluated Nuclear Data File (ENDF) at Brookhaven National Laboratory using calculations based on models for the structure of liquid H_2O and D_2O at several temperatures.

The models for H_2O at elevated temperatures are simple modifications of the MR (McMurry-Russell) model for 22°C water which gives computed scattering in agreement with Brugger's MTR data. The models for D_2O are obtained by scaling the MR model to correspond with using the mass of the D atom in describing the vibrational frequencies and modes in D_2O . For each temperature parameters have been adjusted to optimize agreement with available data.

The data calculated for ENDF are obtained directly from calculations using the models, except in regions where the $S(\kappa^2, \beta)$ vs β functions show sharp spikes due to transitions associated with the characteristic vibrations present in the models. This structure may not be realistic, and may present problems of interpolation in the use of the ENDF data. Therefore, a procedure for calculating smoothed $S(\kappa^2, \beta)$ data in such regions is described.

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PREPARATION OF H_2O AND D_2O SLOW NEUTRON SCATTERING
KERNELS FOR ENDF USING MR TYPE MODELS

I. The Evaluated Nuclear Data File (ENDF)

The Evaluated Nuclear Data File was set up at Brookhaven National Laboratory by Honeck and his collaborators¹ to store nuclear data needed in reactor physics calculations in readily accessible form. Several aims appear to be in view.

1. Selection of standard formats for data storage. Those submitting data can then put it into an immediately usable form, and users will know how to construct their own retrieval routines.

2. Development of retrieval routines, and in some cases, development of programs which compute parameters needed in reactor physics calculations from stored data.

The "evaluated data" in the file are not all evaluated in the sense of being of known accuracy or reliability. In some cases, such as scattering kernels for moderators, such evaluation may have to await the experience of users who make calculations using sets of data from several sources.

In any event, data are stored as discrete values of some function, and appropriate interpolation formulae are available to supply intermediate values when they are needed in calculations.

The philosophy under which ENDF operates is discussed fully in Ref. (1) which also supplies information as to the forms in which data are to be submitted. Ultimately ENDF will probably contain a special file of recommended or reference data (ENDF B). This is not of any concern to this report.

II. The MR Model for H_2O at $295^\circ K$, and Related Models for H_2O at $423^\circ K$ and $550^\circ K$, and for D_2O at $295^\circ K$ and $423^\circ K$

This report describes the procedure used to prepare scattering kernels for H_2O and D_2O for the ENDF file. As explained in Part I, the kernels are calculated from models of the structure of water designed to give agreement with experimental double differential scattering cross sections.

The first of these models², denoted by MR (for McMurtry-Russell), applies to room temperature water. It treats water as a mixture of 10 percent of free H_2O molecules together with 45 percent each of two aggregates in which the effective masses for scattering by H atoms are 75 and 150, respectively. Each aggregate has a set of vibrations with characteristic energies below 0.025 eV in which the vibration amplitudes are chosen so the modes arise from interaction of translational motions of the molecules in the aggregate. Another set of modes with characteristic energies E_r in the range $0.025 < E_r < .125$ eV have amplitudes such that they correspond to interaction of rotational oscillations of the H_2O molecules about their principal axes of inertia.

The parameters in the models³ for water at $423^\circ K$ and $550^\circ K$ are the same as in the MR model except that agreement with Haywood's scattering data⁴ at $423^\circ K$ and Page's data⁵ at $550^\circ K$ has been optimized by choosing the free molecule percentages to be 25 and 28 percent, respectively.

In the D_2O models⁶ the characteristic energies E_r associated with translational oscillations of the molecules are the same as in the MR model, while those associated with rotational oscillations are

reduced by $1/\sqrt{2}$ of their values in the MR model to reflect the effect of the larger mass of the D atoms. The vibration amplitudes have been adjusted so the modes with energies below 0.025 eV correspond to modes involving D_2O translational motions, while those with energies above 0.025 eV involve rotational motions. Seventeen percent of free D_2O molecules was needed to optimize agreement with Haywood's 295°K data⁷, and 53% for the 423°K data.

III. Form of Slow Neutron Scattering Data For ENDF

A. Quantities Needed in Reactor Physics Calculations

Reactor physics calculations require Legendre moments $\int_{-1}^1 \sigma(E_0, E, \mu) P_\ell(\mu) d\mu$ of the double differential scattering cross sections $\sigma(E_0, E, \mu)$ of the materials in the reactor. In some cases the double differential scattering cross sections themselves may be needed. The $\sigma(E_0, E, \mu)$ considered here is for an isotropic scattering system and σ is the cross section for scattering of a thermal neutron from energy E_0 into unit energy range around E , and into unit solid angle about a direction θ with the initial direction. The $\mu = \cos \theta$. Units are barns/eV x sr x group, where "group" may mean "atom", "molecule" or some molecular group such as CH_2 in polyethylene. The Legendre moments which are of interest in reactor physics calculations are defined by

$$\sigma_\ell(E_0, E) = \int_{-1}^1 \sigma(E_0, E, \mu) P_\ell(\mu) d\mu$$

and

$$\sigma_\ell(E_0) = \int_0^\infty \sigma_\ell(E_0, E) dE$$

B. Scattering Functions For ENDF Input

It is convenient to store slow neutron scattering data in the ENDF in the form of either the Egelstaff Scattering Law (ESL)⁸ or as Reduced Partial Differential Scattering Cross Sections (RPDC)^{2,9}, and to obtain the $\sigma_{\ell}(E_0, E)$, $\sigma_{\ell}(E_0)$ and other quantities by operating on the ESL or RPDC functions. For isotropic systems these functions are even in the energy transfer $E - E_0$ and this makes for some simplifications in the data storage.

The ESL function is denoted by $S(\alpha, \beta)$ and is defined by

$$S(\alpha, \beta) = \left[\frac{E_0}{E} \right]^{\frac{1}{2}} e^{\beta/2} \frac{4\pi}{\sigma_b} kT \sigma(E_0, E, \mu) \quad (1)$$

The RPDC is denoted by $S(\kappa^2, \beta)$ and is defined more simply by

$$S(\kappa^2, \beta) = \left[\frac{E_0}{E} \right]^{\frac{1}{2}} e^{\beta/2} \sigma(E_0, E, \mu) \quad (2)$$

These functions are related by

$$S(\alpha, \beta) = \frac{4\pi}{\sigma_b} \cdot kT S(\kappa^2, \beta) \quad (3)$$

In Eqs. (1,2)

$$\beta = (E - E_0)/kT$$

$$|\kappa| \hbar = \text{momentum change of the neutron}$$

$$\alpha = \frac{\kappa^2 \hbar^2}{2MkT} ; \text{ Here } M \text{ is arbitrary but is usually the mass of the most important scattering atom.}$$

$$\sigma_b = \text{bound atom scattering cross section of the principal scatterer (barns)}$$

Units are usually such that kT and other energies are in eV, κ^2 is $\text{\AA}^{-2}$ and masses are in AMU. The units for $S(\kappa^2, \beta)$ are the same as for σ ,

i.e., barns/eV x sr x group. The units for $S(\alpha, \beta)$ are simply per steradian since the barns/group x eV is extracted in the factor $4\pi kT/\sigma_b$.

In some cases it may be desirable to store $S(\kappa^2, \epsilon)$ where $\epsilon = E - E_0$. Experience will probably lead to favoring one form of scattering function, but it is likely that the function will be simply related to those in Eqs. (1,2).

At present data in ENDF are stored as a matrix in which the elements are values of $S(\alpha_j, \beta_i)$ for pairs α_j (or κ_j^2) and β_i of the variables α (or κ^2) and β . The ENDF file has associated with it a retrieval program which computes the Legendre moments and other reactor physics parameters from the stored data. The retrieval program employs a logarithmic interpolation function for expressing the variation of $S(\alpha, \beta)$ between α points and β points.

IV. Method of Calculating Kernels for ENDF

A. Problems Connected with Constructing Slow Neutron Scattering Kernels for ENDF

It would be best to extract $S(\alpha, \beta)$ data for ENDF from experimental slow neutron scattering measurements. This has not been done so far, reliance having been on calculations based on models. The reason is partly that not all experimentalists have geared themselves to supply data in the desired form, but even more because the data do not cover a sufficient range of the variables $\alpha(\kappa^2)$ or β , temperature, and possibly physical structure.

Therefore, up to the present, it has proved expedient to calculate $S(\alpha, \beta)$, or $S(\kappa^2, \beta)$, data from models or in some cases using frequency distributions extracted from the available scattering data.

Some of the methods have been evaluated by comparison with measured $S(\kappa^2, \beta)$ data, others by comparison against angular distributions $\sigma(E_0, \mu)$ vs μ or by comparing measured spectra with calculated spectra.

In the case of kernels calculated for H_2O and D_2O using the MR and related models an additional difficulty arises. When α (or κ^2) is low, the $S(\alpha, \beta)$ vs β curves show sharp resonances whenever $\beta = E_T/kT$, where E_T is one of the characteristic vibrational energies in the model. This behavior is shown in Fig. 1. Experimental data have not been obtained at low enough κ^2 for all β values to reveal whether resonance structure of this type is truly present in water. Since the models oversimplify the structures of liquid H_2O and D_2O it would be misleading to attach physical significance to the details which produce this structure in the calculated $S(\alpha, \beta)$ functions. In addition, the resonances are so sharp that an impractically large number of β_i points might be required to adequately define the function for interpolation by the retrieval routines used in ENDF.

To avoid producing calculated data which might give users an erroneous picture of the structure of water, and to determine an $S(\alpha, \beta)$ function more suited to interpolation by ENDF, an option has been provided for supplying $S(\alpha, \beta)$ data in which the resonances have been "smoothed" out.

B. Calculation of Data for ENDF from the MR and Related Models

1. The General Equation

The ENDF requires a set of $S(\kappa_j^2, \beta_i)$. Usually the number of κ_j^2 is of the order of 50 to 80 covering a range something like $0.05 < \kappa_j^2 < 5000 \text{ \AA}^{-2}$. The present work employs 189 β_i values.

The computing program calculates $S(\kappa_j^2, \beta_i)$ from

$$S(\kappa_j^2, \beta_i) = \sum_v f_v S_v(\kappa_j^2, \beta_i) \quad (4)$$

Here f_v is the fraction of atoms of type v in the scattering system. The ENDF file uses $S(\alpha_j, \beta_i)$ as defined in Eq. (3), but these are readily obtained from the $S(\kappa_j^2, \beta_i)$.

2. Criteria For Smoothing

In most of the space spanned by κ_j^2 and β_i the direct output calculated from Eq. (4) is used for ENDF. Resonances are smoothed only if the following conditions are satisfied.

a. $\kappa_j^2 \leq \kappa_{\max}^2$. Here $\kappa_{\max}^2$ is determined from study of $S(\kappa_j^2, \epsilon_i)$ vs ϵ_i curves and is chosen such that little resonance structure appears if $\kappa_j^2 > \kappa_{\max}^2$. The variable ϵ instead of $\beta = \epsilon/kT$ has been used since resonances come at the same ϵ regardless of T .

b. $\epsilon_i \leq \epsilon_b$ where ϵ_b is an upper value for the energy transfer. The value is arbitrary but the assumption is made here that for water $\epsilon_b < 0.2$ eV. This insures that the internal H_2O modes with characteristic energies of 0.2 and 0.46 eV (two modes) are always calculated exactly. This is because these modes have a clear physical significance. In D_2O this $\epsilon_b < .15$ eV, the energy of the lowest internal mode of D_2O .

c. If $\epsilon_i < \epsilon_{\min}$ no smoothing is used. Here $\epsilon_{\min} \approx .015$ eV. This is done because the resonances with $\epsilon_i < 0.015$ eV are never sharp because the scattering by the free molecules tends to dominate in this region. The same limit can be used in D_2O since the low modes in D_2O are about the same as in H_2O .

d. A minimum $\kappa_{\min}^2$ is determined such that for $\kappa_j^2 < \kappa_{\min}^2$ there is smoothing in the range $\epsilon_{\min} < \epsilon_i < \epsilon_b$. For

$\kappa_{\min}^2 < \kappa_j^2 < \kappa_{\max}^2$, the smoothing range in ϵ decreases as κ_j^2 increases as determined by the curve in Figure 2.

3. The Smoothing Function

In the region of κ^2, β space where smoothing is required, the $S(\kappa_j^2, \beta_i)$ values for ENDF are computed from the functions

$$S(\kappa_j^2, \beta_i) = S_I(\kappa_j^2) e^{-C_I x_i} ; 0 \leq x_i \leq \beta_{I+1/2} - \beta_{I-1/2} \quad (5)$$

The following notation has been adopted in Eq. (5). Capital subscripts I denote quantities associated with resonances. Thus $\beta_I = \epsilon_I/kT$ where ϵ_I is an energy transfer which coincides in value with one of the characteristic energies in the scattering system.

The energy transfers $\beta_{I-1/2}$ and $\beta_{I+1/2}$ denote values midway between β_I and β_{I-1} , and β_I and β_{I+1} , respectively. The remaining energy transfers β_i which do not fall in coincidence with characteristic vibrational energies, or half way between these energies, are subscripted with lower case i .

In Eq. (5), the $S_I(\kappa_j^2)$ and $C_I(\kappa_j^2)$ pertain to the resonance at β_I . The value of $S_I(\kappa_j^2)$ is chosen, if possible, so that $S(\kappa_j^2, \beta_i)$ is a continuous function at $\beta_{I+1/2}$, while $C_I(\kappa_j^2)$ is chosen so that the area under the resonance

$$\phi_I(\kappa_j^2) = \int_{\beta_{I-1/2}}^{\beta_{I+1/2}} S(\kappa_j^2, \beta) d\beta \quad (6)$$

is the same as that which would be calculated from the model without using smoothing. However the higher moments $\int S(\kappa_j^2, \beta) \beta^n d\beta$ may be

somewhat in error.*

The function assumed in Eq. (5) is adapted to the logarithmic interpolation used by the ENDF retrieval program.

4. Method of Calculation of $S_I(\kappa_j^2)$ and $C_I(\kappa_j^2)$ in Eq. (5)

The procedure to be described now for determining the $S_I(\kappa_j^2)$ and $C_I(\kappa_j^2)$ in Eq. (5) assumes that the ϵ or β table includes all the E_r or β_r (which are denoted as in Eq. (5) by E_I or β_I) and values half way between resonances (denoted by $\epsilon_{I+1/2}$ or $\beta_{I+1/2}$). The computing program has been adapted so a table of ϵ values can be inserted. These are converted to β values when $S(\kappa_j^2, \beta_I)$ is calculated. Insertion of an ϵ table means that changes in temperature can be made with assurance that any β_I values used in the calculations have the correct resonance values.

The smoothing calculation begins with the computations of the areas $\phi_I(\kappa_j^2)$ associated with the resonances. The ϕ_I is for the I th resonance. Eq. (6) defines $\phi_I(\kappa_j^2)$. The $\phi_I(\kappa_j^2)$ are computed using the $S(\kappa_j^2, \beta_I)$ values obtained from the computing program for each

*Eq. (5) does not give an $S(\kappa_j^2, \beta_I)$ which is even in β . However, in using the scattering law, values of $S(\kappa^2, \beta)$ are given for positive β and are assumed in the computation to be valid also for negative β . A representation like (5) is valid if this is done. In fact, if (5) were written so that $\beta_{I+1/2}^2$ and β^2 appeared, the logical recipe for choosing the associated C_I would lead to a variation in β over small β intervals which is close to that found from Eq. (5). Eq. (5) is a useful form because it presents $\ln S(\kappa_j^2, \beta_I)$ as a linear function of β_I , and the constant $S_I(\kappa_j^2)$ is given by an analytical equation.

$\beta_i = \epsilon_i/kT$ in the range $\beta_{I-1/2} \leq \beta_i \leq \beta_{I+1/2}$. This is done using numerical integration, or by an asymptotic formula in a way to be described later.

The calculations of the $S_I(\kappa_j^2)$ and $C_I(\kappa_j^2)$ begin at the first resonance $I = 1$. For this resonance $S_1(\kappa_j^2)$ is taken to be the value of $S(\kappa_j^2, \beta_{1-1/2})$ calculated from the MR model unless this value is too low to permit construction of the function in Eq. (5). This case will be discussed below after the "normal" situation is explained.

Once $C_1(\kappa_j^2)$ is obtained, the $C_I(\kappa_j^2)$ is chosen so that Eq. (6) gives the correct area $\phi_I(\kappa_j^2)$. This requires for any ϕ_I except the last

$$\phi_I(\kappa_j^2) = \frac{S_I(\kappa_j^2)}{C_I(\kappa_j^2)} \left[1 - e^{-C_I X_I} \right] \quad (7)$$

$$X_I = \beta_{I+1/2} - \beta_{I-1/2}$$

A value of $C_I(\kappa_j^2)$ satisfying Eq. (7) is found by iteration.

Except for the last resonance, the $S_I(\kappa_j^2)$ and $C_I(\kappa_j^2)$ for the other resonances with $I > 1$ proceed in the same way. The $S_I(\kappa_j^2)$ is obtained from S_{I-1} and C_{I-1} using

$$S_I(\kappa_j^2) = S_{I-1}(\kappa_j^2) \left[1 - e^{-C_{I-1} X_{I-1}} \right] \quad (8)$$

This process is subject to one restriction. If any $S_I(\kappa_j^2)$ is too low compared to $S(\kappa_j^2, \beta_i)$ calculated from the model, the $C_I(\kappa_j^2)$ required to satisfy the area equation, Eq. (7), can become negative and of such large magnitude that $|C_I|X_I$ can exceed 88. This is too large an exponent for the IBM 7040 to calculate, and even if it did the resulting $S(\kappa_j^2, \beta_i)$ function would oscillate wildly.

Therefore, if any $S_I(\kappa_j^2) < 0.1 S(\kappa_j^2, \beta_i)$, the substitution $S_I(\kappa_j^2) = 0.1 S(\kappa_j^2, \beta_i)$ is made to provide a value for use in Eq. (5). Here $S(\kappa_j^2, \beta_i)$ is the value calculated from the model. This results in discontinuities in the smoothed $S(\kappa_j^2, \beta_i)$ vs β_i curves, but the mathematical elaboration required to eliminate these seems unwarranted.

The process outlined above is modified slightly for the last resonance in the smoothing region. The requirement here is to produce an $S(\kappa_j^2, \beta_i)$ vs β_i which is continuous at the β value which bounds the smoothing region.

The functional form used is

$$S = S_I \left[1 - \frac{x}{X_I} \right] e^{-C_I x} + S_b \frac{x}{X_I} e^{C_I (x - X_I)} \quad (9)$$

This requires

$$\begin{aligned} \phi_I = S_I \frac{(1 - e^{-C_I X_I})}{C_I} - \frac{S_I}{X_I C_I^2} \left[1 - (1 + C_I X_I) e^{-C_I X_I} \right] \\ - \frac{S_b}{C_I^2 X_I} \left[1 - C_I X_I - e^{-C_I X_I} \right] \end{aligned} \quad (10)$$

In Eqs. (9,10) the subscript I denotes the resonance in the smoothing regions nearest to $\beta_b = \epsilon_b/kT$. The $S_b(\kappa_j^2)$ is the value of $S(\kappa_j^2, \beta_b)$ computed from the MR model for $\beta = \beta_b = \epsilon_b/kT$. The $C_I(\kappa_j^2)$ is found by iteration. Also, β_b plays the role of $\beta_{I+1/2}$.

5. Calculation of $\phi_I(\kappa_j^2)$ in Eq. (5)

When κ_j^2 is sufficiently low, it is often possible to calculate $\phi_I(\kappa_j^2)$ from a simple analytical formula and thus avoid time consuming numerical integrations. This is possible when $S(\kappa_j^2, \beta)$ near

a resonance is dominated by processes involving excitation of a single quantum of vibrational energy. Under these conditions, $S(\kappa_j^2, \beta)$ can be approximated for H_2O (an analogous equation holds for D_2O) by

$$S(\kappa_j^2, \beta) = f_{HI} S_{HI}(\kappa_j^2, \beta) + f_{OI} S_{OI}(\kappa_j^2, \beta) \quad (11)$$

In Eq. (11), $f_{HI} = 2f_{OI}$, and f_{OI} is the fraction of H_2O molecules which are in the aggregate containing the mode with characteristic energy E_I . (No characteristic energy in the range $0 < E_I < 0.125$ eV is in more than one aggregate.) The S_{HI} and S_{OI} are the contributions to $S(\kappa_j^2, \beta)$ from the H atom and O atom, respectively. Near the resonance the equation for $S_{HI}(\kappa_j^2, \beta)$ is approximately given by

$$S_{HI}(\kappa_j^2, \beta) = \frac{\sigma_{bH}}{4\pi} \cdot \frac{1}{2kT\sqrt{\bar{\alpha}_H}} \cdot \frac{\bar{g}_{HI}}{2} e^{-\left(\sum_{\tau} \bar{g}_{H\tau} \cosh(\beta_{\tau}/2)\right)} e^{-\left(\frac{[\bar{\alpha}_H^2 + (\beta - \beta_{\tau})^2]}{4\bar{\alpha}_H}\right)} \quad (12)$$

In Eq. (12)

σ_{bH} = bound atom scattering cross section for H

$\bar{\alpha}_H = \frac{\kappa_H^2}{2M_{HI}} \cdot \frac{1}{kT}$; M_{HI} = effective scattering mass for an H atom in the aggregate which has the characteristic energy E_I .

$$\bar{g}_{HI} = \frac{\kappa_H^2 \bar{e}_{HI}}{6E_I \sinh(\beta_I/2)} = \frac{\kappa^2}{1448} \frac{\bar{e}_{HI} m}{E_I \sinh(\beta_I/2)} \quad (13)$$

In Eq. (13), $\frac{\bar{e}_{HI}}{E_I}$ is proportional to the mean squared displacement

$\langle \Delta r_{HI}^2 \rangle$ of the H atom during execution of the normal mode with

characteristic energy E_I . The m is the neutron mass in atomic units.

The sum $\sum_{\tau} \bar{g}_{H\tau} \cosh(\beta_{\tau}/2)$ is over all modes in the scattering aggregate

which are given a quantum treatment. The S_{OI} is computed from the

same type of equation except that parameters for the O atom appear.

When Eq. (12) represents the scattering, the $\phi(\kappa_j^2, \beta_I)$ is given by

$$\phi(\kappa_j^2, \beta_I) = f_{HI} \phi_H(\kappa_j^2, \beta_I) + f_{OI} \phi_O(\kappa_j^2, \beta_I) \quad (14)$$

$$\phi_H(\kappa_j^2, \beta_I) = \frac{\alpha_{bH}}{4\pi kT} \frac{\bar{g}_{HI}}{2} \exp - \left[\sum_{\tau} \bar{g}_{H\tau} \cosh(\beta_{\tau}/2) + \frac{\bar{\alpha}_H}{4} \right] \quad (15)$$

The $\phi_O(\kappa_j^2, \beta_I)$ is calculated from an equation like (15) except that parameters for the O atom are used.

In practice $\phi_H(\kappa_j^2, \beta_I)$ contributes almost all to Eq. (14). The computation scheme involves procedures for treating a mode classically whenever the energy transfer exceeds the characteristic energy sufficiently. The criteria are such that, in some cases, the mode with energy E_I will be treated quantum mechanically in S_{HI} and classically in S_{OI} . In such cases, the oxygen contribution to Eq. (14) is omitted.

The program decides whether to compute $\phi_I(\kappa_j^2)$ by Eq. (15), by first determining the ratios $\frac{S(\kappa_j^2, \beta_{I-1/2})}{S(\kappa_j^2, \beta_I)}$ and $\frac{S(\kappa_j^2, \beta_{I+1/2})}{S(\kappa_j^2, \beta_I)}$.

If the largest ratio is less than some fractional number G_4 , it uses Eq. (15). Otherwise, it computes $\phi_I(\kappa_j^2)$ by numerical integration. In practice G_4 as high as 0.5 seems feasible.

V. Some Results

Table I lists the 189 ϵ_I values used in making calculations on H_2O . Those ϵ_I which correspond with values equal to characteristic vibrational energies are underlined twice, while the $\epsilon_{I+1/2}$ which are midway between the ϵ_I are underlined once. This Table has been used for all H_2O temperatures. Figure 1 displays some results.

Table I

Characteristic Energies ϵ_i for H_2O *

.000	<u>.00038</u>	.00075	.00125	.00188	.00250	.00375
<u>.00500</u>	.00600	<u>.00650</u>	.00700	<u>.00750</u>	.00825	<u>.00900</u>
.00950	<u>.01000</u>	.01050	.01100	<u>.01150</u>	.01200	<u>.01250</u>
.01300	.01350	<u>.01400</u>	.01450	<u>.01500</u>	.01550	.01600
<u>.01650</u>	.01700	<u>.01750</u>	.01800	.01850	<u>.01900</u>	.01950
<u>.02000</u>	.02050	.02100	<u>.02150</u>	.02200	<u>.02250</u>	.02300
.02350	<u>.02400</u>	.02450	<u>.02500</u>	.02625	.02750	.02875
.03000	<u>.03125</u>	.03250	.03375	.03500	.03625	<u>.03750</u>
.03875	.04000	.04125	.04250	<u>.04375</u>	.04500	.04625
.04750	.04875	<u>.05000</u>	.05125	.05250	.05375	.05500
<u>.05625</u>	.05750	.05875	.06000	.06125	<u>.06250</u>	.06375
.06500	.06625	.06750	<u>.06875</u>	.07000	.07125	.07250
.07375	<u>.07500</u>	.07625	.07750	.07875	.08000	<u>.08125</u>
.08250	.08375	.08500	.08625	<u>.08750</u>	.08875	.09000
.09125	.09250	<u>.09375</u>	.09500	.09625	.09750	.09875
<u>.10000</u>	.10125	.10250	.10375	.10500	<u>.10625</u>	.10750
.10875	.11000	.11125	<u>.11250</u>	.11375	.11500	.11625
.11750	<u>.11875</u>	.12000	.12125	.12250	.12375	<u>.12500</u>
.12625	.12750	.13000	.13250	.13500	.13750	.14375
.15000	.16250	<u>.17500</u>	.18000	.18250	.18500	.18750
.19000	.19250	.19500	.19750	<u>.20000</u>	.20250	.20500
.20750	.21000	.21250	.21875	.22500	.23750	.25000
.27500	.30000	.33750	.37500	.41250	.42500	.43125
.43750	.44375	.45000	.45625	<u>.46000</u>	.46875	.47500
.50000	.55000	.60000	.65000	.72500	.80000	.87500
.95000	1.05000	1.10000	1.17500	1.25000	1.32500	1.40000
1.50000	1.65000	1.80000	1.95000	2.10000	2.25000	2.38000

* Double underlines denote ϵ_I values coinciding with characteristic vibrational energies; single underlines denote $\epsilon_{I+1/2}$, usually half way between ϵ_I .

Table II lists the 67 κ_j^2 values which have been used for both H_2O and D_2O at all temperatures.

Table II

<u>The κ_j^2 Values</u>						
.05000	.06513	.08200	.10320	.13000	.16360	.20600
.25940	.32660	.41110	.51760	.65170	.82050	1.03300
1.30100	1.63700	2.06100	2.59500	3.26800	4.11400	5.17900
6.52100	8.21000	10.34000	13.01000	16.38000	20.63000	25.97000
32.69000	41.16000	51.82000	65.25000	82.14000	103.40000	130.20000
163.90000	206.40000	259.80000	300.00000	350.00000	411.90000	450.00000
518.50000	600.00000	700.00000	821.90000	900.00000	1035.00000	1200.00000
1400.00000	1640.00000	1800.00000	2065.00000	2200.00000	2400.00000	2600.00000
2800.00000	3000.00000	3200.00000	3400.00000	3600.00000	3850.00000	4121.00000
4370.00000	4600.00000	4850.00000	5189.00000			

The program for calculating the $S(\kappa_j^2, \beta_i)$ data for input to ENDF is based on one¹⁰ which calculates $S(\kappa^2, \beta)$, $\sigma(E_O, E, \mu)$ and moments of the form $\sigma_\ell(E_O, E) = \int_{-1}^1 \sigma(E_O, E, \mu) P_\ell(\mu) d\mu$ for molecules in which vibrational energy transfers may be important. Descriptions of the input requirements and output formats are available.¹¹

Figure 1

Unsmoothed and Smoothed MR Model $S(\kappa^2, \epsilon)$ vs ϵ functions for $0.025 \leq |\epsilon| \leq 0.095$ and $\kappa^2 = 1.0$ and $4.1 \text{ \AA}^{-2}$. Arrows indicate $\epsilon_{I+1/2}$ points. Note that, except for the discontinuity at $|\epsilon| = 0.0325$ and $\kappa^2 = 1.0$, the curves are continuous at the $\epsilon_{I+1/2}$ although the slopes are discontinuous.

Figure 2

Region of κ^2 , $|\epsilon|$ space in which $S(\kappa^2, \epsilon)$ is smoothed

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9. R. M. Brugger, "Compilation of Reduced Slow Neutron Partial Differential Scattering Cross Sections," IDO-16699(Rev.), Phillips Petroleum Company, Idaho Falls, Idaho (1962).

10. H. L. McMurry and L. J. Gannon, "A Machine Method for Calculating Slow Neutron Scattering with Application to Water," IDO-16984, Phillips Petroleum Company, Idaho Falls, Idaho (1964). In Eq. (33) the factor multiplying $1/(1+4a)$ should be $1-[1+(1+4a)\beta^2]^{\frac{1}{2}}$. On p. 18 the proper definition of $\alpha_{\max}$ is

$$\alpha_{\max} = \frac{-1}{b} + \frac{1}{b} [1+b\beta^2]^{\frac{1}{2}}$$

$$b = 1 + 4M_v \left[\sum_{\tau} \frac{\bar{\delta}_{v\tau}}{3\beta_{\tau}} \coth (\beta_{\tau}/2) \right]$$

11. The input and output for the program which calculates smoothed $S(\kappa^2, \beta)$ data for ENDF is described in the Phillips Petroleum Company Computing Center (Idaho Falls, Idaho) program description PPCo 40.0652. The input-output for the program described in Ref. 10 is given in Ref. 10, but an up-dated version is presented in the Phillips program description PPCo 40.0828. These descriptions are available on request.